spack

building models better

ACCESS
Australian Earth System Simulator
National Research Infrastructure
access-nri.org.au

Reliable and Reproducible: Building Models Better With Spack

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Current

What you get

autotools
CMake Meson
CachedCMake
Python
SCons
Waf Lua
Octave Perl
Racket SIP
R QMake
Ruby
ROCm module
Apache Maven

Imagine being given a box of mixed LEGO and trying to build a model with only some of the instructions and not all the right pieces.

Building scientific models is similar: with the current mix of build systems it's hard to find exactly the pieces you need, they often aren't available, so you have to make do, and the pieces don't seem to fit together well.

Spack finds all the pieces, builds the dependencies and then then model and writes detailed instructions so it can build exactly the same model again, and again and again.

Spack is a build from source package manager that makes building reliable and reproducible.

FUJITSU intel Google Cloud
aws arm NVIDIA

What you want

Reproducible builds: means variation in model output is due to factors under **your** control, not changes in dependencies or build tools

This is **CRITICAL**

Developed at LLNL

7000 packages

1100 contributors

Popular and widespread

Spack

SIP
Python
ROCm
autotools
SCons
QMake
module
CMake
Meson
Racket
R
CachedCMake
Apache Maven

spack wraps build systems making them interoperable

What you get

Highly expressive syntax allows for complete customisation of builds including compiler and dependency versions.

```
spack install access-om2 %intel@2021.1.2 ^nci-openmpi@4.0.2
    ^netcdf-c@4.7.4 ^netcdf-fortran@4.5.2
```

Same recipe can be used to build a model on an HPC, a GitHub runner, inside a container or on your laptop.

```
docker build -f Dockerfile.base-spack -t spack-dev:latest --target=dev .
docker run -it --rm spack-dev:latest
```

Automatic dependency resolution: finds all dependencies listed in your build. All dependencies must be spack packages.

Spack will build your model and it's dependencies for you, and can write a full spack.lock file that records all aspects of the build, giving full build provenance.

From a lockfile spack can reproducibly rebuild your model, ensuring build reproducibility.

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